Neutron Matter with Auxiliary Field Diffusion Monte Carlo

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Introduction

We want to solve for the eigenstates of A nonrelativistic neutrons (and nucleons) interacting with a spin-isospin dependent potential. I'll show results for the equation of state and spin susceptibility of neutron matter, and show some calculations of the energy gap at low density.

Outline of talk

- Description of the nuclear Hamiltonian we use.

- Description of the auxiliary field diffusion Monte Carlo method.

- The path constraint

- Some results for neutron matter.

- Future directions and conclusions

Hamiltonian

The Hamiltonian is

$$H = \sum_i \frac{p_i^2}{2m_i} + \sum_{i<j} \sum_{p=1}^{M} v_p(r_{ij}) O^{(p)}(i,j) + V_3$$

where i and j label the two nucleons, r_{ij} is the distance separating the two nucleons, and the $O^{(p)}$ include spin, isospin, and spin orbit operators, and M is the maximum number of operators (i.e. 18 in Argonne v_{18} model).

We use the Argonne v_8' potential. For neutrons isospin exchange gives the identity. The terms are central, spin-exchange, tensor, and spin-orbit.

The Urbana and Illinois three-body potentials for neutrons have a two-body spin structure of this same type where the third particle is a spectator that changes only the strength of the interaction.

The central Part can be handled using standard GFMC or DMC.

The most successful method for light nuclei uses Monte Carlo for central part and complete summation over the spin-isospin states.

The number of good S_z T_z spin-isospin states is

$$\frac{A!}{Z!(A-Z)!}2^A$$

which can be lowered by a small factor if good T^2 states are constructed.

The exponential growth of these states limits this brute force method to around 14 to 16 neutrons.

Diffusion Monte Carlo for Central Potentials

Schrödinger equation in imaginary time (measured in units of energy^{-1}) is the diffusion equation

$$(H - E_T)\Psi(R, t) =$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(R) - E_T \right]\Psi(R, t) = -\frac{\partial}{\partial t}\Psi(R, t)$$

Formal solution

$$\Psi(R, t) = e^{-(H - E_T)t}\Psi(R, 0)$$
$$H\Psi_n(R) = E_n\Psi_n(R)$$
$$\Psi(R, 0) = \sum_n a_n\Psi_n(R)$$
$$\Psi(R, t) = e^{-(E_0 - E_T)t}a_0\Psi_0(R)$$
$$+ \sum_{n \neq 0} e^{-(E_n - E_0)t}a_n\Psi_n(R)$$

Result converges to the lowest energy eigenstate not orthogonal to $\Psi(R, 0)$.

Short time Approximation

For short time propagation:

$$e^{-H\Delta t} = e^{-V\frac{\Delta t}{2}} e^{-\frac{P^2}{2m}\Delta t} e^{-V\frac{\Delta t}{2}} + O(\Delta t^3)$$

In R representation the $P^2/2m$ term is the free propagator, and the V terms are diagonal,

$$G(R, R', \Delta t) = \langle R|e^{-(H-E_T)\Delta t}|R'\rangle$$

$$= \left[\frac{1}{2\pi\sigma^2}\right]^{\frac{3A}{2}} e^{-\frac{(R-R')^2}{2\sigma^2}} e^{-[\frac{V(R)+V(R')}{2} - E_T]\Delta t}$$

$$\sigma^2 = 4\frac{\hbar^2}{2m}\Delta t$$

Monte Carlo Algorithm

The algorithm for equal mass particles is

1. Sample walker R_i positions from $\Psi(R,0)$. Each walker has weight 1.

2. Add Gaussian random variate with variance σ^2 to each coordinate.

3. The walker weight becomes $W_i = e^{-[\frac{V(R_i)+V(R_i')}{2}-E_T]\Delta t}$ where R_i and R_i' are the new and old positions.

4. Change W to an integer N_i by $N_i = \mathrm{int}(W_i + \xi)$, ξ is a random variate uniformly distributed on $(0,1)$. Take N_i copies of the new position R_i.

5. Repeat steps 2-4.

6. Calculate mixed expectation values from

$$O_{\mathrm{mixed}} = \frac{\sum_i \Psi_T^*(R_i)O(R_i)}{\sum_i \Psi_T(R_i)}$$

Additional Items

- Use importance sampling to decrease variance. Sample instead from approximations to

$$\frac{\Psi_T(R)}{\Psi_T(R')}G(R, R', \Delta t)\,.$$

and solve for

$$\Psi_T(R)\Psi(R, t)$$

- For fermion problems, the wave function is not positive everywhere. Either use fixed node approximation or transient estimation.

Monte Carlo Spin-Isospin Sampling

We want to sample the spins, but current good wave functions require the same computational effort to calculate First look in the usual n↑, n↓ basis.

$R \equiv 3A$ x, y, z coordinates for the nucleons

$S \equiv A$ discrete values selecting one of n↑, n↓

$\Psi_T(R, S) =$ Trial wavefunction - a complex number for given R and S.

$H_{S,S'}(R) =$ the Hamiltonian

There are 2^A spin states. We could sample them with low variance if we could calculate $\Psi_T(R, S)$ efficiently.

All known nontrivial trial functions require order 2^A operations to calculate either 1 or all the spin states.

Auxiliary Field Motivation

The idea is to apply auxiliary fields and constrained path ideas of

S. Zhang, J. Carlson, and J. Gubernatis, Phys. Rev. Lett **74**, 3652 (1995), Phys. Rev. **B55**, 7464 (1997),

to the spin-isospin part of the Nuclear Hamiltonian, while sampling the spatial part as in Green's function or Diffusion Monte Carlo.

See: S. Fantoni, A. Sarsa, and K.E. Schmidt, Phys. Rev. Lett. **87** , 181101 (2001). K.E. Schmidt and S. Fantoni, Phys. Lett. **446**, 99 (1999).

- We need to sample the spin states to do large A systems.

- Sampling in the S_z, T_z basis gives high variance unless a good trial function is used. Current good trial functions are too expensive to use for large A systems.

Our Auxiliary Field Choice

We diagonalize the interaction in spinor space. This requires Order(A^3) operations, but the trial wave function determinant has the same complexity. This breakup is similar to those used in auxiliary field break ups in Shell Model Monte Carlo.

For A particles, the spin-spin interaction can be written as

$$
\begin{aligned}
V &= V_c + V_{nc} \\
&= V_c + \frac{1}{2} \sum_{i,\alpha,j,\beta} \sigma_{i,\alpha} A_{i,\alpha,j,\beta} \sigma_{j,\beta}
\end{aligned}
$$

- The A matrix is zero when $i = j$ and symmetric.

- The A matrix is real and symmetric and has real eigenvalues and eigenvectors.

- The eigenvectors and eigenvalues are defined by

$$
\sum_{j,\beta} A_{i,\alpha,j,\beta} \psi_{j,\beta}^{(n)} = \lambda_n^{(\sigma)} \psi_{i,\alpha}^{(n)}
$$

The matrix can be written in terms of its eigenvectors and eigenvalues to give the noncentral potential

$$V_{nc} = \frac{1}{2} \sum_{n,i,\alpha,j\beta} \sigma_{i\alpha} \psi_{i\alpha}^{(n)} \lambda_n \psi_{j\beta}^{(n)} \sigma_{j\beta} = -\frac{1}{2} \sum_n v_n^2$$

$$v_n = \sum_{i,\alpha} \sqrt{-\lambda_n} \psi_{i\alpha}^{(n)} \sigma_{i\alpha}$$

The Hubbard-Stratonovich transformation is

$$e^{-V\Delta t} \simeq \prod_n \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dy_n e^{\frac{-y_n^2}{2}} e^{y_n v_n \sqrt{\Delta t}}$$

The y_n variables are the auxiliary fields. The integral is done using Monte Carlo. For a selected y_n value, the resulting operator rotates spinors, but leaves the Monte Carlo sample as an outer product of spinors times a delta function in space.

Spin-orbit is in this linear form in the spinors and can be done similarly.

Constrained Path

- We still have the usual fermi sign problem, in this case the overlap of our walkers with the trial function will be complex.

- We constrain the path to regions where the real part of the overlap with our trial function is positive.

- For spin independent potentials this reduces to the fixed-node approximation.

Application to Neutron Matter

- Here we use the simplest trial function

$$|\Psi_T\rangle = \left[\prod_{i<j} f_{ij}^c\right] A \left[\prod_i |\phi_i, s_i >\right]$$

- The overlap is the determinant of the space-spin orbitals evaluated at the walker position and spinor for each particle multiplied by a central Jastrow product.

- For neutron matter in a box of side L, the orbitals are plane waves that fit in the box times up and down spinors.

- Usual closed shells for each noninteracting spin state contain 1,7,19,27,33,57 ... particles
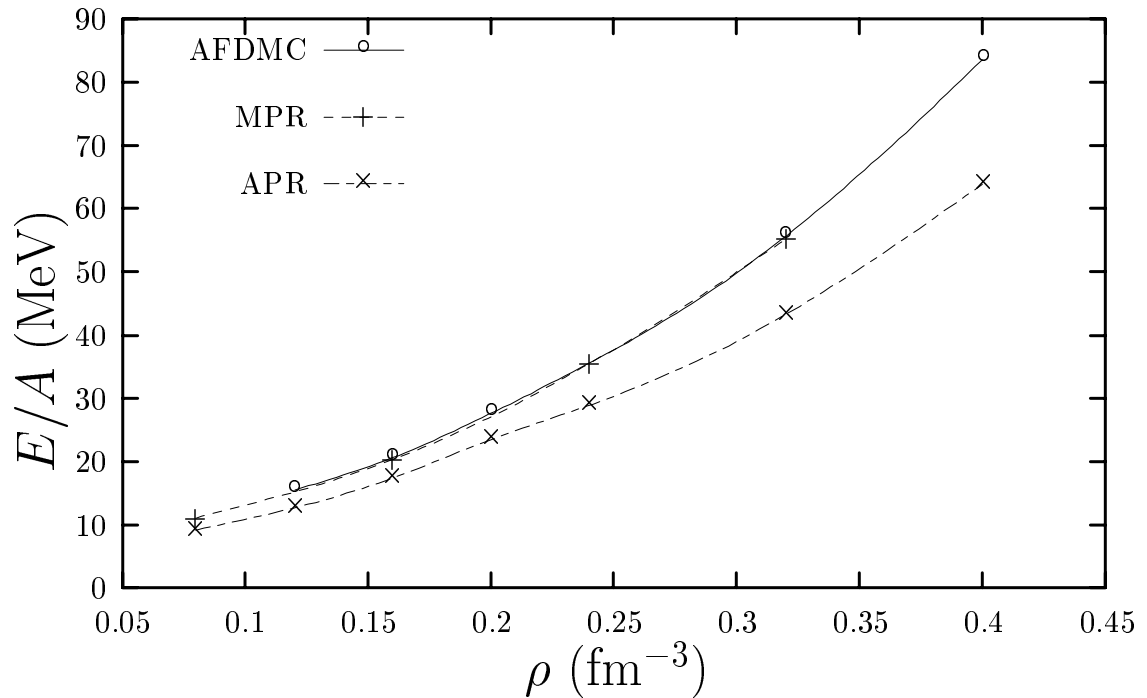
v$'_8$ Neutron Matter equation of State
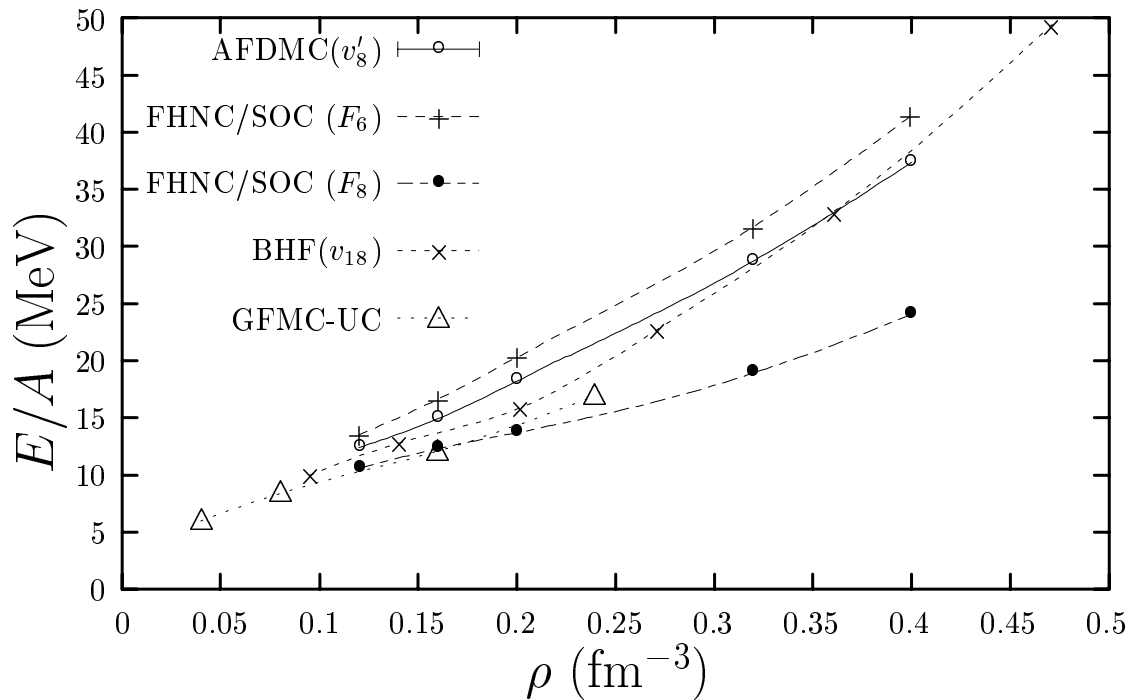
AFDMC energy per particle for neutron matter with the v'_8 potential. Variational FHNC/SOC results obtained with correlation functions of type F_6 and F_8 along with the the extrapolated Green's function Monte Carlo [†] and Brueckner-Hartree-Fock[‡].

[†]J. Carlson, J. Morales, Jr., V. R. Pandharipande and D. G. Ravenhall, *Quantum Monte Carlo calculations of neutron matter*,nucl-the/0303041 (2003).

[‡]M. Baldo, G. Giansiracusa, U. Lombardo and H. Q. Song, *Bethe-Brueckner-Goldstone expansion in neutron matter*, Phys. Lett. B **473**, 1 (2000).

# $\mathbf{v'_8 + UIX}$ Neutron Matter equation of State

Extrapolated AFDMC Equation of state of pure neutron matter with the $AU8'$ potential. The variational results of APR [†] and MPR [‡] corresponding to the Argonne v_{18} two body plus Urbana IX three body potential are also plotted.

[†]A. Akmal,V. R. Pandharipande and D. G. Ravenhall, *Equation of state of nucleon matter and neutron star structure*, Phys. Rev. C **58** (1998) 1804.

[‡]J. Morales, Jr., V. R. Pandharipande, and D. G. Ravenhall, *Improved variational calculations of nucleon matter*, Phys. Rev. C **66**, 054308 (2002).

v_8', Urbana IX, Transient Estimate

$$\rho = 0.32 \text{ Fm}^{-3}$$

Neutron Matter Transient Estimate
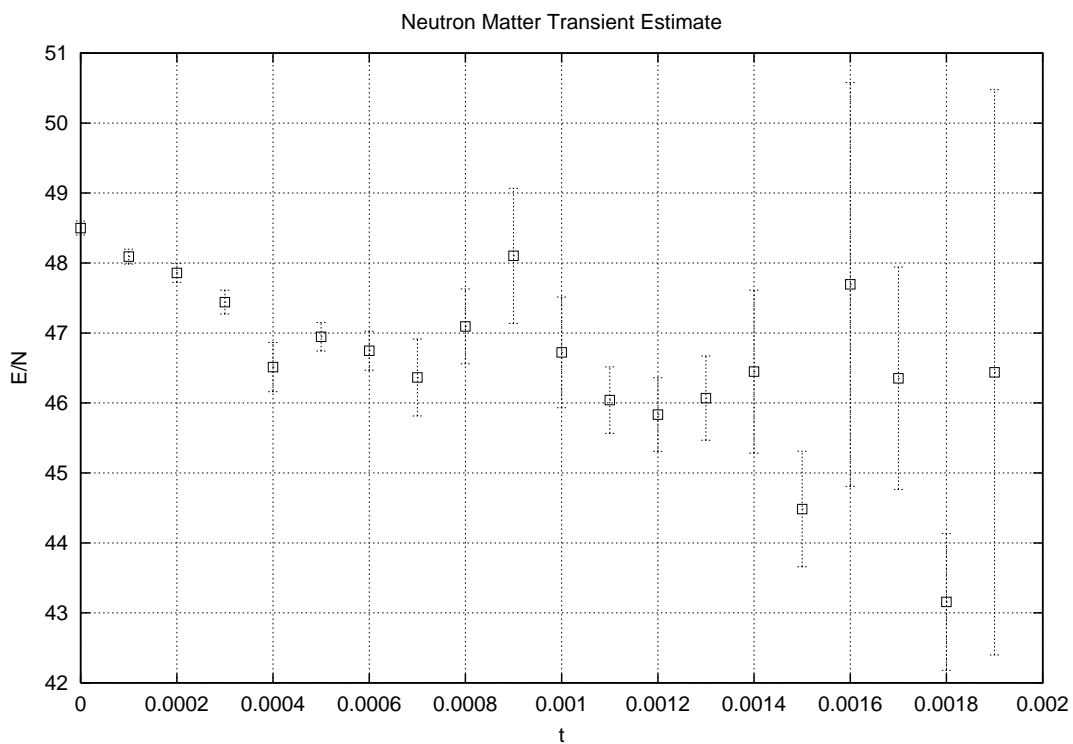
Spin Susceptibility

The spin susceptibility and corresponding response functions can be related to the neutrino cross sections in neutron matter. These cross sections have important implications for the dynamics of supernovae.

The long wave length static response can be calculated from the energy. Adding a magnetic field, the spin response is described by

$$
\begin{aligned}
H &= H_0 - \sum_i \vec{\sigma}_i \cdot \vec{b} \\
\vec{b} &= \mu \vec{B} \\
\mu &= 6.03 \times 10^{-18} \text{ MeV/Gauss}
\end{aligned}
$$

The spin susceptibility is

$$
\chi = -n\mu^2 \left. \frac{\partial^2 E_0(b)}{\partial b^2} \right|_{b=0}
$$

where $E_0(b)$ is the ground state energy in the field b.

The spin polarization with the field along $\hat{z}$ is $p = \langle \sigma_z \rangle$. Using AFDMC we can calculate $E_0(J_z, b)$ within the constrained path approximation. Using the chain rule, we can write
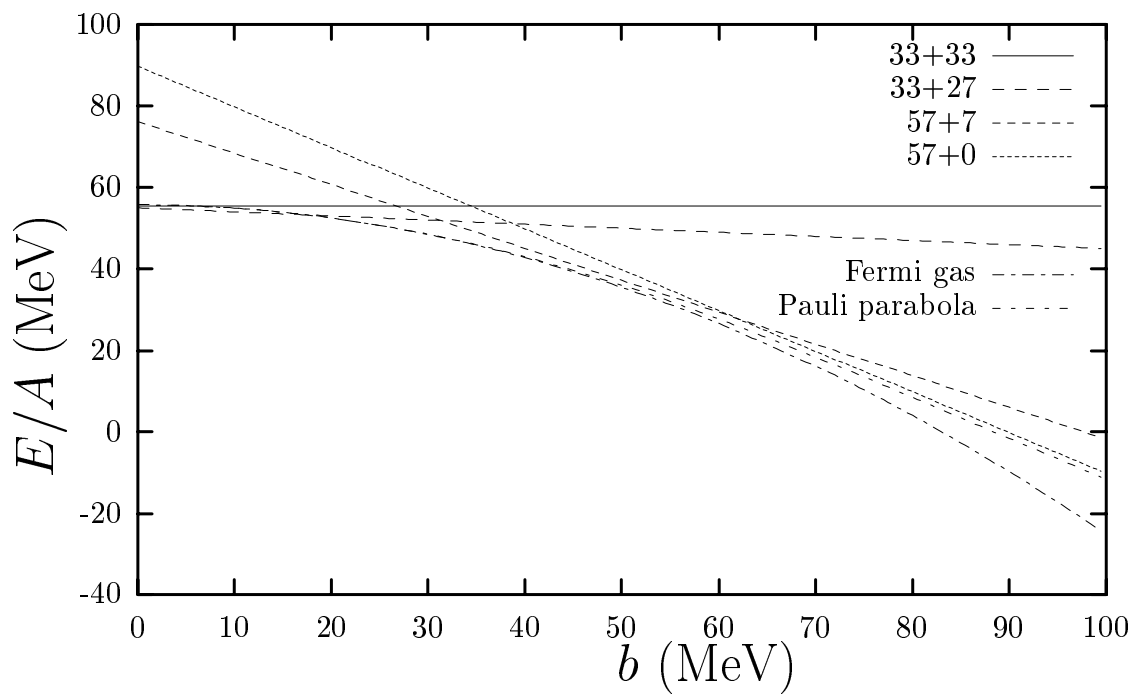
$$\frac{\chi}{\chi_{\text{Pauli}}} = \frac{\hbar^2 k_f^2 \left(\frac{\partial p}{\partial b}\right)^2}{3m\frac{\partial E}{\partial J_z^2}}$$

and

$$p(J_z) = -\left.\frac{\partial E_0(b, J_z)}{\partial b}\right|_{b=0}$$

Noninteracting Energy with magnetic field

The energy of noninteracting neutrons as a function of magnetic field at $\rho = 0.32$ fm^{-3} for various finite sized close shell trial functions with spin up and down values shown. Also plotted is the correct infinite system energy and the parabolic Pauli estimate.

NonInteracting Susceptibility

The susceptibility χ of non–interacting fermions obtained by assuming that the energies are quadratic in b, and normalized to the exact Fermi free gas value χ_F.
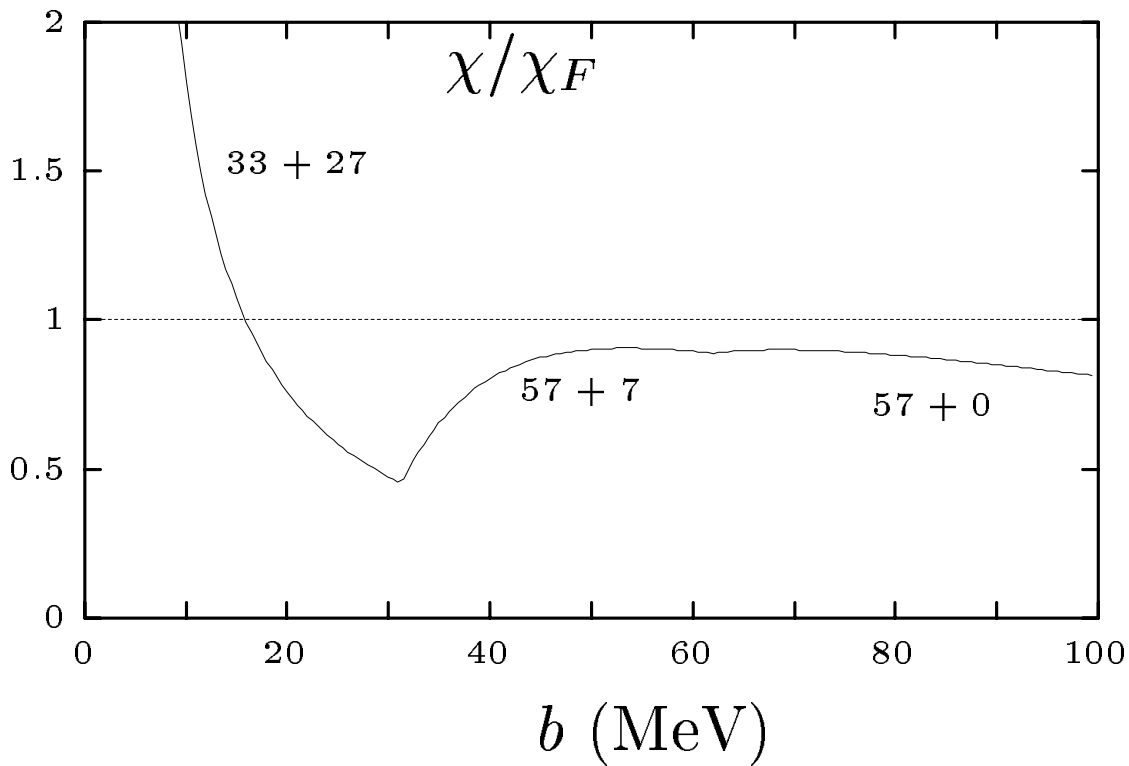
Calculation of Susceptibility

Assuming:

$E_0(J_z)$ is quadratic in J_z even at $57\uparrow + 7\downarrow$,

$p(J_z)$ is linear in J_z even at $57\uparrow + 7\downarrow$,

Energy is linear in b even at 50 MeV.

Compressibility

ρ/ρ_0	Reid[†]	Reid6[‡]	AU18[§]	AU6-CBF[¶]	AU6'
0.75	0.91	2.06	1.10	0.85	0.89(3)
1.25	0.70	1.35	0.71	0.45	0.47(3)
2.0	0.49	0.77	0.26	0.23	0.21(3)
2.5	0.42	0.60	0.15	0.17	0.14(3)

Compressibility ratio $\mathcal{K}/\mathcal{K}_F$ of neutron matter. The AFDMC results for the AU6' interaction are compared with other calculations. The statistical error is given in parentheses.

[†]Brueckner calculations by S. O. Bäckmann and C. G. Källman, Phys. Lett. B **43** (1973) 263.

[‡]CBF calculations by A. D. Jackson, E. Krotscheck, D. E. Meltzer and R. A. Smith, Nucl. Phys. A **386** (1992) 125.

[§]FHNC calculations of A. Akmal, V. R. Pandharipande and D. G. Ravenhall, Phys. Rev. C **58** (1998) 1804.

[¶]CBF calculations of A. Fabricini, private communication.

Spin Susceptibility

ρ/ρ_0	Reid[†]	Reid6[‡]	AU6'	AU8'	Reid6
0.75	0.45	0.53	0.40(1)		
1.25	0.42	0.50	0.37(1)	0.39(1)	0.36(1)
2.0	0.39	0.47	0.33(1)	0.35(1)	
2.5	0.38	0.44	0.30(1)		

Spin susceptibility ratio χ/χ_F of neutron matter. The AFDMC results for the interactions AU6', AU8' and Reid6 are compared with those obtained from the Landau parameters calculated from FHNC and CBF theories. The statistical error is given in parentheses.
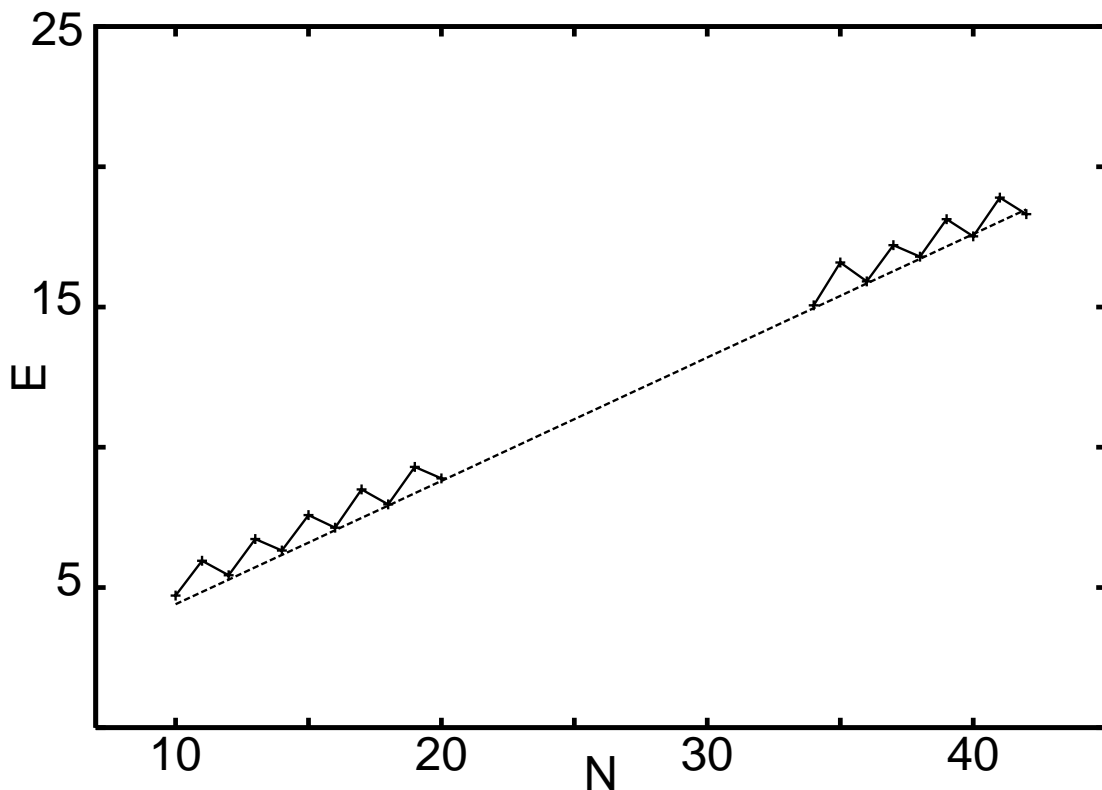

[†]Brueckner calculations by S. O. Bäckmann and C. G. Källman, Phys. Lett. B **43** (1973) 263.

[‡]CBF calculations by A. D. Jackson, E. Krotscheck, D. E. Meltzer and R. A. Smith, Nucl. Phys. A **386** (1992) 125.

Pairing Results

We want to examine the effect of BCS pairing at low densities.
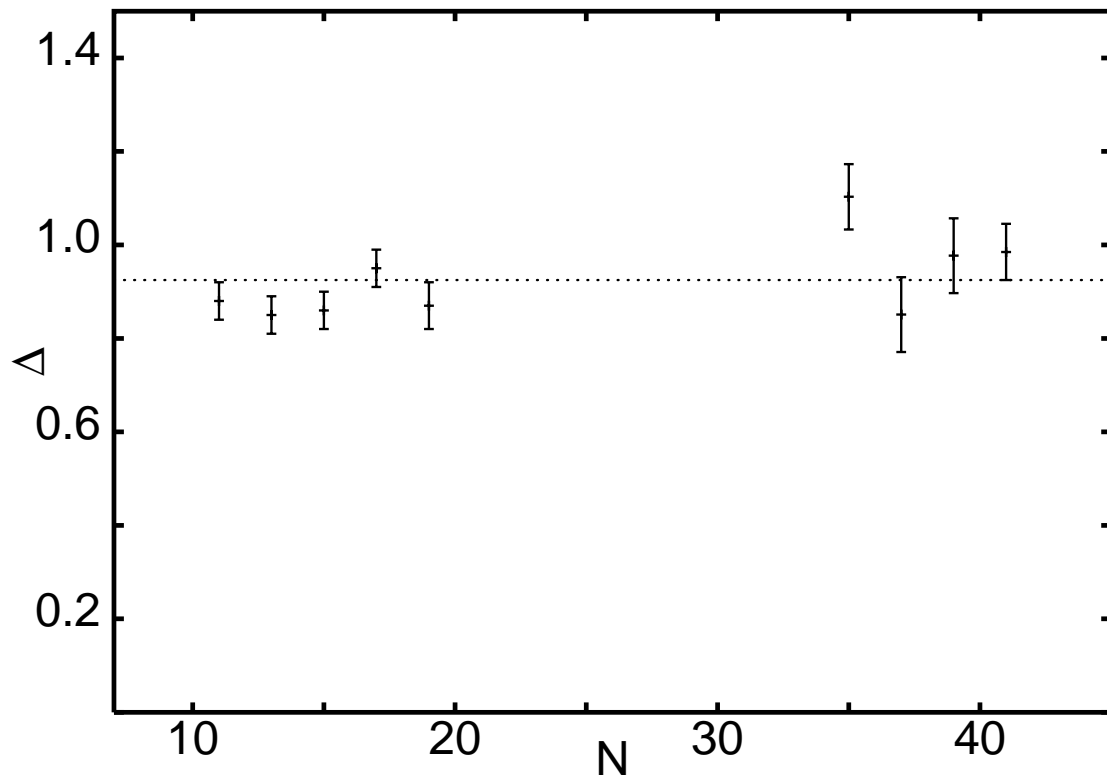
Use a BCS nodal constraint for a short range infinite scattering length central potential [†]

Energy in units of free gas energy, as a function of particle number. Notice no shell effects.

[†]J. Carlson, S-Y Chang, V.R. Pandharipande, K.E. Schmidt, *Superfluid fermi gases with large scattering length*, physics/0303094.

Even-Odd Energy Gap

Energy Gap $\Delta = E(N) - \frac{1}{2}[E(N+1) + E(N-1)]$ for N odd. in units of the free gas energy per particle.

Pairing in Neutron Matter

The general pairing form becomes the Pfaffian of a skew symmetric matrix rather than a determinant.

A general state with n paired and o unpaired orbitals for a total of $N = 2n + o$ particles can be written as

$$\mathcal{A}[\phi_{12}\phi_{34}...\phi_{2n-1,2n}...\psi_1(2n+1)...\psi_o(N)]$$

which is the pfaffian of the $(N+o) \times (N+o)$ matrix

$$\begin{pmatrix}
0 & \phi_{12} & \phi_{13} & \cdots & \phi_{1N} & \psi_1(1) & \cdots & \psi_o(1) \\
-\phi_{12} & 0 & \phi_{23} & \cdots & \phi_{2N} & \psi_1(2) & \cdots & \psi_o(2) \\
-\phi_{13} & \phi_{23} & 0 & \cdots & \phi_{3N} & \psi_1(3) & \cdots & \psi_o(3) \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
-\phi_{1N} & -\phi_{2N} & -\phi_{3N} & \cdots & 0 & \psi_1(N) & \cdots & \psi_o(N) \\
-\psi_1(1) & -\psi_1(2) & -\psi_1(3) & \cdots & -\psi_1(N) & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
-\psi_o(1) & -\psi_o(2) & -\psi_o(3) & \cdots & -\psi_o(N) & 0 & \cdots & 0
\end{pmatrix},$$

where the lower $o \times o$ section is all zeroes.

Pfaffian can be calculated efficiently.
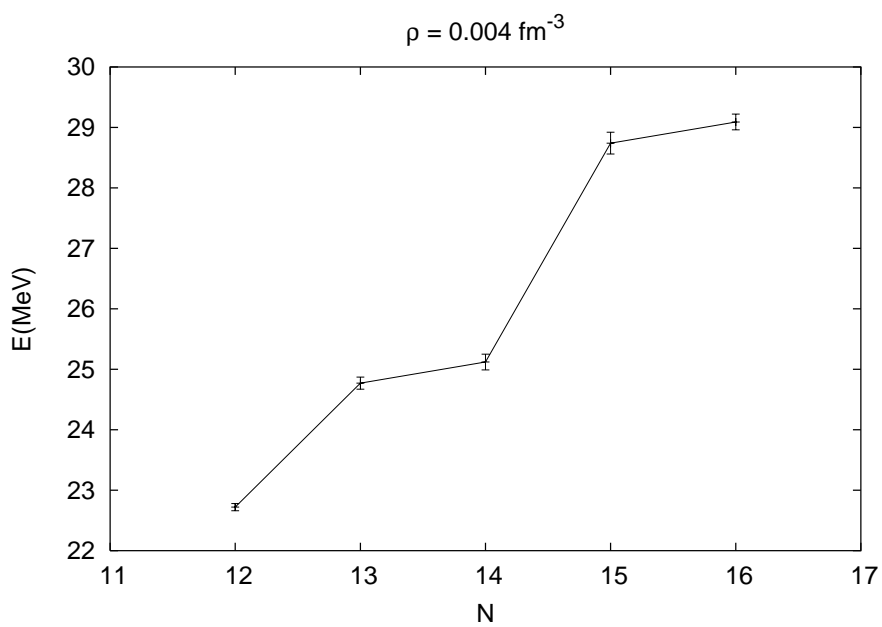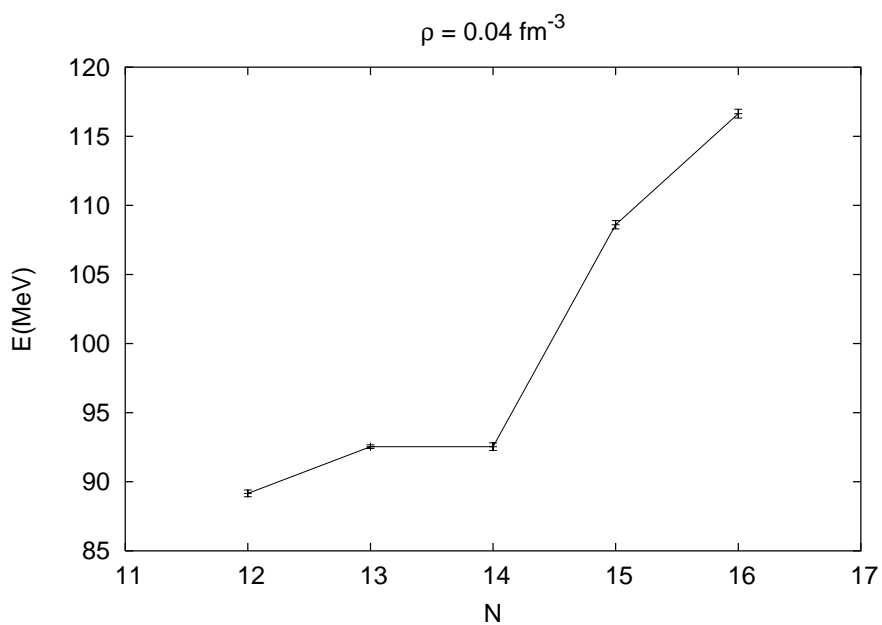
Pairing Results in Neutron Matter

$\rho = 0.04$, paired open shell trial function.

N	E/N	E	Δ
12	7.43 (2)	89.16 (24)	—
13	7.15 (1)	92.54 (13)	1.7(2)
14	6.61 (2)	92.54 (28)	—
15	7.24 (2)	108.60 (30)	4.0(4)
16	7.29 (2)	116.64 (32)	—

$\rho = 0.004$, paired open shell trial function.

N	E/N	E	Δ
12	1.893(5)	22.72(6)	—
13	1.905(8)	24.77(10)	0.85(12)
14	1.794(9)	25.12(13)	—
15	1.916(12)	28.74(18)	1.64(20)
16	1.818(8)	29.09(13)	—

Neutron Matter Pairing Energies

$\rho = 0.04$ fm^{-3}

$\rho = 0.004$ fm^{-3}

Conclusions

We have a method for approximately calculating the properties of large A nuclear systems with Monte Carlo and are approaching what are considered realistic interactions.

Future Plans

1. Complete BCS gap calculations.

2. Investigate pion condensate in neutron matter.

3. Add protons to neutrons.

4. Mesons, Nucleons, Response functions ...